

Supporting Information

Regulating anti-thermal quenching to zero thermal quenching for highly efficient blue-emitting Eu²⁺-doped K-beta-alumina phosphors

Yuhang Kuang,^a Yunjia Li,^a Borui Chen,^a Shujuan Zhao,^a Mengfang Chen,^a Shixun Lian,^a Jilin Zhang^{*a}

^a Key Laboratory of Light Energy Conversion Materials of Hunan Province College, Key Laboratory of Chemical Biology and Traditional Chinese Medicine Research (Ministry of Education of China), Hunan Normal University, Changsha 410081, China

*Email: chemzhangjl@hunnu.edu.cn

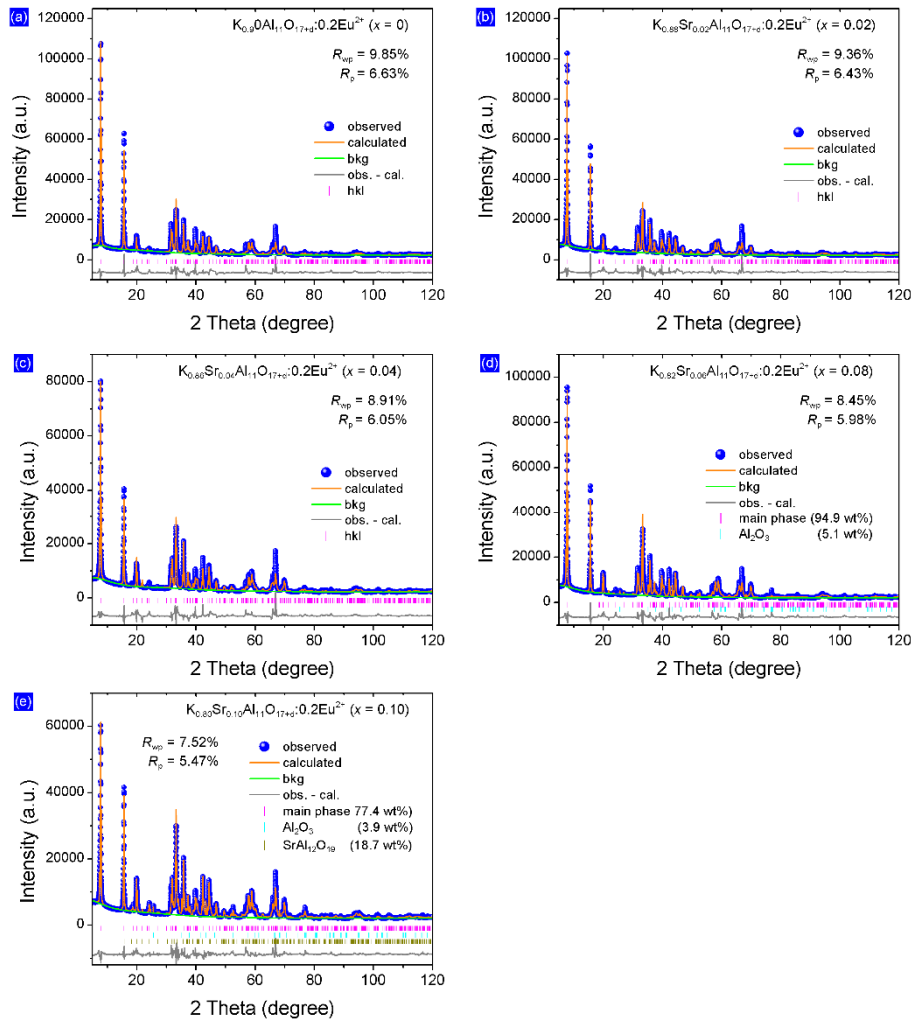


Figure S1. Rietveld refinement results for $K_{0.90-x}Sr_xAl_{11}O_{17+d}:0.2Eu^{2+}$. (a) $x = 0$, (b) $x = 0.02$, (c) $x = 0.04$, (d) $x = 0.08$, (e) $x = 0.10$.

Table S1. Cell parameters of $K_{0.90-x}Sr_xAl_{11}O_{17+d}:0.2Eu^{2+}$ ($x = 0.06$)

| Atom | Wyck. | Site | $x / \text{\AA}$ | $y / \text{\AA}$ | $z / \text{\AA}$ | S.O.F | $U_{iso} / \text{\AA}^2$ |
|------|-------|------|------------------|------------------|------------------|--------|--------------------------|
| K1 | 6h | mm2 | 0.66732 | 0.33463 | 1/4 | 0.222 | 0.0098 |
| Sr1 | 6h | mm2 | 0.66732 | 0.33463 | 1/4 | 0.01 | 0.0098 |
| Eu1 | 6h | mm2 | 0.66732 | 0.33463 | 1/4 | 0.0444 | 0.0098 |
| K2 | 6h | mm2 | 0.88396 | 0.76791 | 1/4 | 0.058 | 0.0098 |
| Sr2 | 6h | mm2 | 0.88396 | 0.76791 | 1/4 | 0.01 | 0.0098 |
| Eu2 | 6h | mm2 | 0.88396 | 0.76791 | 1/4 | 0.0222 | 0.0098 |
| Al1 | 12k | m | 0.83143 | 0.66287 | 0.10856 | 0.9837 | 0.0065 |
| Al2 | 4f | 3m | 1/3 | 2/3 | 0.02840 | 1 | 0.0111 |
| Al3 | 4f | 3m | 1/3 | 2/3 | 0.17066 | 0.9294 | 0.0024 |
| Al4 | 2a | -3m | 0 | 0 | 0 | 1 | 0.0211 |
| O1 | 12k | m | 0.15747 | 0.31495 | 0.05328 | 1 | 0.0064 |
| O2 | 12k | m | 0.50196 | 0.00393 | 0.14264 | 1 | 0.0122 |
| O3 | 4f | 3m | 2/3 | 1/3 | 0.04890 | 0.9354 | 0.0127 |
| O4 | 4e | 3m | 0 | 0 | 0.14287 | 1 | 0.0322 |
| O5 | 6h | mm2 | 0.30183 | 0.60366 | 1/4 | 0.333 | 0.0489 |

Table S2. Cell parameters of $K_{0.90-x}Sr_xAl_{11}O_{17+d}:0.2Eu^{2+}$

| | $a / \text{\AA}$ | $c / \text{\AA}$ | $V / \text{\AA}^3$ |
|------------|------------------|------------------|--------------------|
| $x = 0$ | 5.597(1) | 22.685(1) | 615.45(4) |
| $x = 0.02$ | 5.600(1) | 22.690(1) | 616.26(4) |
| $x = 0.04$ | 5.608(1) | 22.718(1) | 618.65(4) |
| $x = 0.06$ | 5.603(1) | 22.696(1) | 616.99(3) |
| $x = 0.08$ | 5.605(1) | 22.706(1) | 617.74(3) |
| $x = 0.10$ | 5.598(1) | 22.680(1) | 615.55(4) |

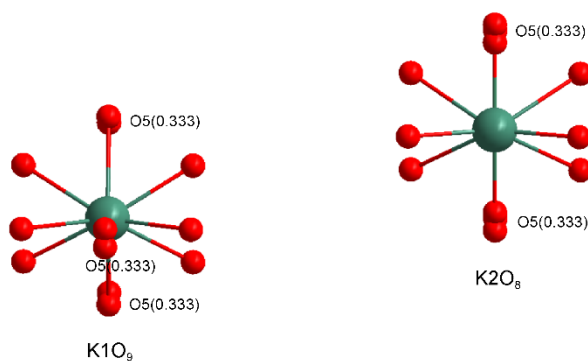


Figure S2. K1O₉ and K2O₈ polyhedrons.

Table S3. K-O bond lengths (Å) for $\text{K}_{0.90-x}\text{Sr}_x\text{Al}_{11}\text{O}_{17+d}\cdot 0.2\text{Eu}^{2+}$

| | K1-O2(x6) | K1-O5(x3) | <i>D</i> of K1 | K2-O2(x4) | K2-O4(x2) | K2-O5(x2) |
|-----------------|------------------------------|--|----------------|-----------|-----------|-----------|
| <i>x</i> = 0 | x4: 2.862(1) x2: 3.020(1) | x2: 2.984(1) x1: 3.288(1) | 0.03277 | 3.083(1) | 2.688(1) | 2.557(1) |
| <i>x</i> = 0.02 | x4: 2.874(1) x2: 2.919(1) | x2: 3.112(1) x1: 3.196(1) | 0.03753 | 3.093(1) | 2.677(1) | 2.776(1) |
| <i>x</i> = 0.04 | x4: 2.946(1) x2: 2.959(1) | x2: 3.125(1) x1: 3.149(1) | 0.02696 | 3.140(1) | 2.642(1) | 2.660(1) |
| <i>x</i> = 0.06 | x4: 2.912(1) x2: 2.918(1) | x2: 3.090(1) x1: 3.100(1) | 0.02680 | 3.093(1) | 2.680(1) | 2.559(1) |
| <i>x</i> = 0.08 | x4: 2.837(1) x2: 3.008(1) | x1: 3.025(1) x1: 3.047(1) x1: 3.335(1) | 0.04111 | 3.075(1) | 2.637(1) | 2.648(1) |
| <i>x</i> = 0.10 | x4: 2.906(6) x2: 2.971(8) | x1: 3.052(1) x1: 3.040(1) x1: 3.158(1) | 0.2322 | 3.070(7) | 2.627(10) | 2.546(1) |

The polyhedral distortion index (*D*) can be calculated by the following equation,^[1]

$$D = \frac{1}{n} \sum_{i=1}^n \frac{|l_i - l_{av}|}{l_{av}}$$

where l_i and l_{av} are the single and average bond length for the central atom and coordinating atom(s), respectively.

Table S4. Thickness (Å) of the spinel blocks and K layers*

| | Spinel blocks | K layers |
|-----------------|---------------|----------|
| <i>x</i> = 0 | 6.4833 | 4.8591 |
| <i>x</i> = 0.02 | 6.4675 | 4.8774 |
| <i>x</i> = 0.04 | 6.4841 | 4.8748 |
| <i>x</i> = 0.06 | 6.4850 | 4.8628 |
| <i>x</i> = 0.08 | 6.5422 | 4.8111 |
| <i>x</i> = 0.10 | 6.6136 | 4.7266 |

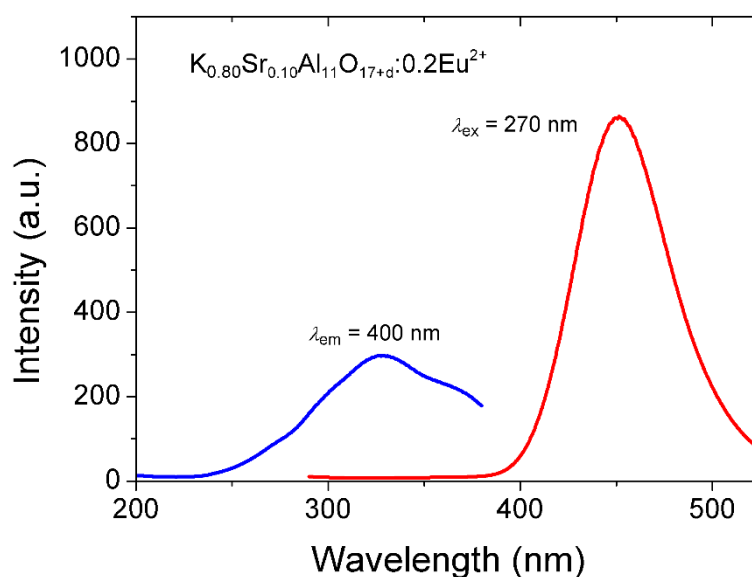


Figure S3. PL ($\lambda_{\text{ex}} = 270 \text{ nm}$) and PLE spectra ($\lambda_{\text{em}} = 400 \text{ nm}$) of $\text{K}_{0.80}\text{Sr}_{0.10}\text{Al}_{11}\text{O}_{17+d}:\text{0.2Eu}^{2+}$.

The $\text{SrAl}_{12}\text{O}_{19}:\text{Eu}^{2+}$ exhibited a PL band at around 400 nm under excitation at 272 nm, according to published literatures.^[2,3] However, $\text{K}_{0.80}\text{Sr}_{0.10}\text{Al}_{11}\text{O}_{17+d}:\text{0.2Eu}^{2+}$ has no PL and PLE spectra that are similar to $\text{SrAl}_{12}\text{O}_{19}:\text{Eu}^{2+}$. This phenomenon indicates that the formation of a small amount of $\text{SrAl}_{12}\text{O}_{19}:\text{Eu}^{2+}$ does not influence the PL profile of $\text{K}_{0.90-x}\text{Sr}_x\text{Al}_{11}\text{O}_{17+d}:\text{0.2Eu}^{2+}$.

[1] X. Zhang, M.-H. Fang, Y.-T. Tsai, A. Lazarowska, S. Mahlik, T. Lesniewski, M. Grinberg, W. K. Pang, F. Pan, C. Liang, W. Zhou, J. Wang, J.-F. Lee, B.-M. Cheng, T.-L. Hung, Y.-Y. Chen, R.-S. Liu, *Chem. Mater.*, 2017, **29**, 6781-6792

[2] R. Zhong, J. Zhang, X. Zhang, S. Lu and X.-j. Wang, *Nanotechnology*, 2007, **18**, 445707.

[3] R. Zhong, J. Zhang, X. Zhang, S. Lu, X. Ren and X.-j. Wang, *J. Phys. D: Appl. Phys.*, 2018, **41**, 065104.